Message

From: Nadine Kotlarz [nkotlar@ncsu.edu]
Sent: 7/26/2018 2:39:02 AM
To: Detlef R. U. Knappe [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=user17c3f77b]
CC: Jane Hoppin [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=userebcfc262]; Adrien Wilkie [aawilkie@ncsu.edu]; McCord, James [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=McCord, James]; Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]
Subject: Re: Serum results update

Hi all,
Looping in Mark and James here to please correct me if I'm wrong.

Background for PFMOAA is very high on the Orbitrap so we could not monitor for it.
The samples do not have 6:2FTS. We did MS/MS to check the fragmentation of what looked like a 6:2FTS peak in the samples and determined it was actually the Nafion byproduct 2 carboxylic acid compound (Hydro-EVE). Therefore, you can disregard the sample concentrations for 6:2FTS. We also detected Hydro-EVE in a few water extracts.
The LOQ for GenX is 10 ppb at best since this is the lowest standard we ran. I am only seeing four samples with concentrations > 10 ppb in the data (797, 471, 790, 396_dup). The other measurement for sample 396 was < 10 ppb, so it's unclear whether it has GenX or not. Therefore, I would say almost all of the samples did not have quantifiable levels of GenX. Yes, I can rerun study IDs 394 and 779. Should we also rerun 797, 471, 790 and 396?

Nadine

On Wed, Jul 25, 2018 at 10:18 AM, Detlef Knappe <knappe@ncsu.edu> wrote:
> Right...
> BTW, the 6:2FtS, might actually another Nafion byproduct carboxylic acids. Nadine mentioned that when she first talked about the results. So my first comment from last night may need to be reassessed.
> Detlef

> On Wed, Jul 25, 2018, 9:51 AM Jane Hoppin <jahoppin@ncsu.edu> wrote:
> The units aren't on the spreadsheet...remember that these values are ppb and the water is ppt.

> On Tue, Jul 24, 2018 at 11:09 PM, Detlef Knappe <knappe@ncsu.edu> wrote:
> Some interesting results here!!!
>
> We never see 6:2 FtS in the water, but it's in the blood! The only location, where we've been able to measure 6:2 FtS in water is near the Greensboro airport. It's source would be related to firefighting training.
>
> Long-chains are readily seen in serum, even if below MRL in water (e.g. PFNA, PFDA, PFO5DoDA)
>
> GenX is present in more than half of the serum samples, some levels quite elevated.
>
> Detection frequency of short-chains is surprisingly high (e.g., PFBA, PFPeA, PFHxA, GenX, PMPA, PEPA), but no PFMOAA.

Hopefully the one PFOS value is not real

Chemours will send us a standard for Nafion BP2-COOH. They call this compound Hydro-EVE

Where comparisons are possible, Wilmington levels > NHANES

On Tue, Jul 24, 2018 at 6:30 PM Adrien Wilkie <aawilkie@ncsu.edu> wrote:

Hi Nadine,

If possible, it would be a good idea to **rerun IDs 394 and 779**.

Thank you for sharing your R code. After reading through it, I realized that 741 had a duplicate that I had not removed. Also, it looks like **366 (in addition to 711)** is missing from the serum data. Does David's inventory not list anything for 366?

Attached are some initial stats generated from the first serum spreadsheet you posted. Please note that the <LOQ was not assigned in its final/correct form.

- tab 1: <[LOQ] values set to missing -- for a preliminary look, all negative values and NF were considered <LOQ
- tab 2: <[LOQ] values set to zero -- for a preliminary look, all negative values and NF were considered <LOQ
- tab 3: quick glance how the two methods change the medians
- tab 4: output of the 10 highest concentrations for each PFAS, then brief counts for which IDs were super high; then the top 10 list sorted by sample ID (Study IDs 779 and 394 are consistently high -- way high.)
- tab 5: NHANES comparison values from the 2013-2014 report

Thanks,
Adrien

Adrien Wilkie, MSPH
Research Assistant
GenX Exposure Study

On Tue, Jul 24, 2018 at 5:30 PM, Jane Hoppin <jahoppin@ncsu.edu> wrote:

Thanks Nadine,

Adrien and I have picked out a few IDs that we think should be rerun. She can send you those.

Also, we've created a different shape table so that we can work with the data...I'll forward it to you. We have 56% with detectable GenX and some are not the ones that are essentially 0, so you may want to take a look.

I hope you are doing well and taking good care of yourself and Roya.

Jane

On Tue, Jul 24, 2018 at 5:21 PM, Nadine Kotlarz <nkotlar@ncsu.edu> wrote:

Jane, Adrien,

Please take a look at the attached data table of serum concentrations (ug/L) for 23 PFAS compounds and the R code I used to create this table. This is as far as I can get today...

A few comments:

1. ISTD means internal standard
2. 6:2FTS_ISTD= 6:2_FTS_ISTD This was just a mistake in the naming. I corrected it in the combined file (along with a few other things I caught) and replaced the file on Google Drive
3. "NF" means that a peak was not found at the specific retention time. You will see "NA" for the calcAmt of internal standards because we did not have calibration curves for the internal standards so concentrations could not be determined.
4. We had standards for all of the analytes except the Nafion byproduct 2 carboxylic acid (i.e., "Nafionbp2COOH"). This compound is very similar in mass and elutes at the same time as 6:2FTS. We can estimate Nafionbp2COOH's concentrations using the 6:2FTS calibration curve (which is how I get the calcAmt values you are seeing in the table) but it would be safer just to report instrument response for this compound.
5. In our next run of serum samples from the May 2018 sampling, do we want to rerun some of the outliers from the November 2017 sampling? (note that PFOS for study ID 394 is > 1000 ug/L).
6. It looks like I am missing results for study ID 711. It was in the SEPA inventory David sent but I don't see it in the Orbitrap results files. I will check into it when I'm back at EPA this week along with throwing out the sample from study ID 710.

Two things that still need work:

1. Apply a threshold area count for each sample so that only samples with responses > 3*noise are considered real values. I think this will take care of the few positive GenX hits we are seeing - I am doubting they are real. Noise would be defined by responses in the calf serum and STD_0.
2. I haven't replaced the negative or low concentrations with "< LOQ." The LOQ for each compound for each run can be determined by looking at the standards. The lowest concentration that is not "excluded" in peakStatus is the LOQ.

Please let me know if you have any questions. If you need a quick response, please give me a call.

Thanks,
Nadine

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